

## HEXAMETHYLENE-1,6-DIISOCYANATE

Hexamethylene-1,6-diisocyanate is a federal hazardous air pollutant and was identified as a toxic air contaminant in April 1993 under AB 2728.

CAS Registry Number: 822-06-0

OCN(CH<sub>2</sub>)<sub>6</sub>NCO

Molecular Formula: C<sub>8</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>

Hexamethylene-1,6-diisocyanate is a colorless to clear liquid with a sharp, pungent odor. It is also combustible (HSDB, 1991).

### Physical Properties of Hexamethylene-1,6-diisocyanate

Synonyms: 1,6-diisocyanatohexane; 1,6-hexamethylene diisocyanate; HDI; hexane1,6-diisocyanate; HMDI

Molecular Weight:	168.22
Boiling Point:	255 °C
Melting Point:	-67 °C
Flash Point:	140 °C (284 °F)
Vapor Density:	5.81 (air = 1)
Density/Specific Gravity:	1.04 at 25/15.5 °C (water = 1)
Vapor Pressure:	0.05 mm Hg at 25 °C
Conversion Factor:	1 ppm = 6.9 mg/m <sup>3</sup>

(HSDB, 1991; Sax, 1987; U.S. EPA, 1994a)

## SOURCES AND EMISSIONS

### A. Sources

Hexamethylene-1,6-diisocyanate is primarily used as a chemical intermediate (HSDB, 1991). The primary stationary sources reporting emissions in California are auto body repair shops, aircraft and parts equipment manufacturing, and the manufacturers of guided missiles and space vehicles (ARB, 1997b).

### B. Emissions

The total emissions of hexamethylene-1,6-diisocyanate from stationary sources in California were at least 300 pounds per year based on data obtained from the Air Toxics "Hot Spots" Program (AB 2588) (ARB, 1997b).

### C. Natural Occurrence

No information about the natural occurrence of hexamethylene-1,6-diisocyanate was found in the readily-available literature.

## AMBIENT CONCENTRATIONS

No Air Resources Board data exist for ambient measurements of hexamethylene-1,6-diisocyanate.

## INDOOR SOURCES AND CONCENTRATIONS

No information about the indoor sources of hexamethylene-1,6-diisocyanate was found in the readily-available literature.

## ATMOSPHERIC PERSISTENCE

Hexamethylene-1,6-diisocyanate will exist in the atmosphere in the gas phase. The dominant atmospheric loss process for hexamethylene-1,6-diisocyanate is expected to be by reaction with the hydroxyl (OH) radical. Based on this reaction, and the using an estimated rate constant from the four  $-CH_2-$  groups, the atmospheric half-life and lifetime of hexamethylene-1,6-diisocyanate is estimated to be less than or equal to 2 days and less than or equal to 3 days, respectively (Atkinson, 1995).

## AB 2588 RISK ASSESSMENT INFORMATION

The Office of Environmental Health Hazard Assessment reviews risk assessments submitted under the Air Toxics "Hot Spots" Program. Of the risk assessments reviewed as of April 1996, hexamethylene-1,6-diisocyanate contributed to the total cancer risk in 1 of the approximately 550 risk assessments reporting a total cancer risk equal to or greater than 1 in 1 million (OEHHA, 1996a).

## HEALTH EFFECTS

Probable routes of human exposure to hexamethylene-1,6-diisocyanate are inhalation and dermal contact.

Non-Cancer: Hexamethylene-1,6-diisocyanate is extremely irritating to the eyes and respiratory tract and can result in respiratory sensitization. Cross-sensitization to other isocyanates can occur. Acute exposure of humans to high concentrations may result in coughing, shortness of breath, and pulmonary edema. There is limited evidence from epidemiologic studies that chronic exposure to hexamethylene-1,6-diisocyanate may cause chronic lung problems in humans, which is often diagnosed as asthma. In animals, chronic inhalation exposure has been

found to result in depressed weight gain, adverse effects on lungs, and organ weight gains in the adrenal glands (U.S. EPA, 1994a).

The Reference Concentration (RfC) for hexamethylene-1,6-diisocyanate is under review by the United States Environmental Protection Agency (U.S. EPA), and an oral Reference Dose (RfD) has not been established (U.S. EPA, 1994a).

No information is available on adverse reproductive or developmental effects of hexamethylene-1,6-diisocyanate in humans or animals (U.S. EPA, 1994a).

Cancer: No information is available on the carcinogenic effects of hexamethylene-1,6-diisocyanate in humans or animals. The International Agency for Research on Cancer and the U.S. EPA have not classified hexamethylene-1,6-diisocyanate for carcinogenicity in humans (IARC, 1987a; U.S. EPA, 1994a).

